

10/552,118

=> d his

(FILE 'HOME' ENTERED AT 10:10:32 ON 07 JUN 2010)

FILE 'REGISTRY' ENTERED AT 10:10:55 ON 07 JUN 2010

L1 682 S CARBODIIMIDE
L2 STRUCTURE UPLOADED
L3 50 S L2
L4 1944 S L2 SSS FUL

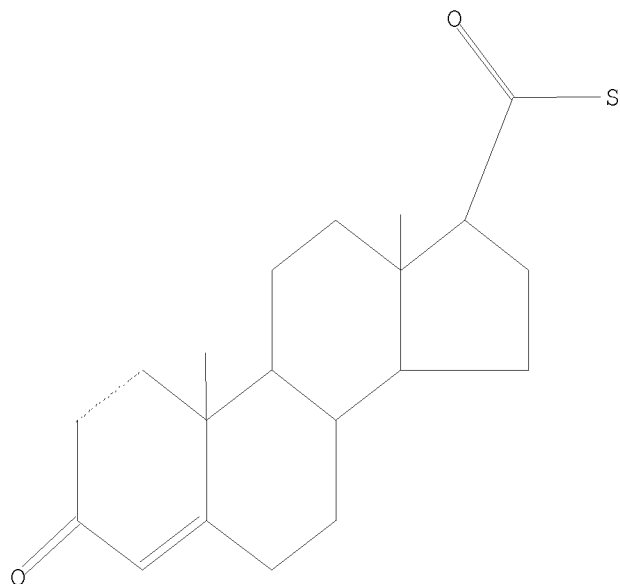
FILE 'CAPLUS' ENTERED AT 10:14:32 ON 07 JUN 2010

L5 2320 S L4
L6 14951 S L1
L7 4 S L5 AND L6

=> d 12

L2 HAS NO ANSWERS

L2 STR



Structure attributes must be viewed using STN Express query preparation.

=> => d ibib abs hitstr total

L7 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2008:252506 CAPLUS

DOCUMENT NUMBER: 148:308571

TITLE: Preparation of uronic acid derivatives as metalloproteinase inhibitors

INVENTOR(S): Sattigeri, Viswajanani J.; Palle, Venkata P.; Khera, Manoj Kumar; Reddy, Ranadheer; Tiwari, Manoj Kumar; Soni, Ajay; Abdul Rauf, Abdul Rehman; Joseph, Sony; Musib, Arpita; Dastidar, Sunanda G.; Srivastava, Punit Kumar

PATENT ASSIGNEE(S): Ranbaxy Laboratories Limited, India

SOURCE: PCT Int. Appl., 183 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

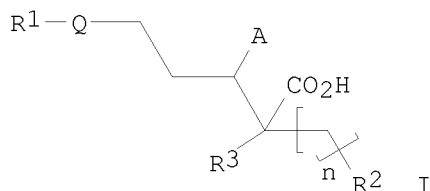
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008023336	A2	20080228	WO 2007-IB53340	20070821
WO 2008023336	A3	20080424		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			
AU 2007287230	A1	20080228	AU 2007-287230	20070821
CA 2661299	A1	20080228	CA 2007-2661299	20070821
EP 2074093	A2	20090701	EP 2007-826082	20070821
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, RS			
JP 2010501545	T	20100121	JP 2009-525162	20070821
MX 2009001963	A	20090330	MX 2009-1963	20090220
IN 2009DN01499	A	20090619	IN 2009-DN1499	20090304
NO 2009001169	A	20090518	NO 2009-1169	20090319
KR 2009053922	A	20090528	KR 2009-705737	20090320
CN 101528691	A	20090909	CN 2007-80038726	20090417
US 20100081610	A1	20100401	US 2009-438182	20091009
PRIORITY APPLN. INFO.:			IN 2006-DE1880	A 20060822
			WO 2007-IB53340	W 20070821

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): CASREACT 148:308571; MARPAT 148:308571

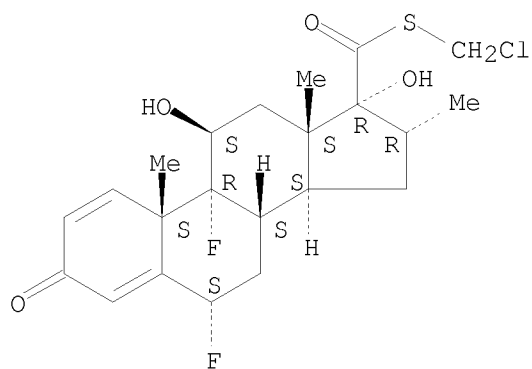
GI



- AB The present invention relates to β -hydroxy and amino substituted carboxylic acids I, wherein n is an integer from 1 to 5; R^1 is H, optionally substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl, heteroaryl, aralkyl, alkoxy, aryloxy, alkenyl-oxy or alkynyl-oxy; R^2 is heterocyclyl, heteroaryl, NR_4R_5 , $-NHC(=Y)R_4$, $-NHC(=Y)NR_5R_x$, $-NHC(O)OR_4$, $-NHSO_4R$ $C(=Y)NR_4R_5$, $C(O)OR_6$, wherein: Y is O or S, OR_5 , $-OC(O)NR_4R_5$, O-acyl, $S(O)mR_4$, $-SO_2N(R_4)_2$, cyanoamidino or guanidine; R_x is R_4 or $-SON(R_4)_2$; R_6 is H, alkyl, cycloalkyl, aralkyl, heteroaryl-alkyl, heterocyclyl-alkyl or cycloalkyl-alkyl, wherein: R_4 is alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl, heteroaryl, aralkyl, heteroaryl-alkyl, heterocyclyl-alkyl or cycloalkyl-alkyl; and m is an integer 0-2; R_5 is H or R_4 ; R_3 is H, fluorine, alkyl, cycloalkyl-alkyl or aralkyl; A is OH, OR_4 , $-OC(O)NR_4R_5$, O-acyl, NH, NR_4R_5 , $-NHC(=Y)R_4$, $-NHC(=Y)NR_5R_x$, $-NHC(O)OR_4$, $-NHSO_2R_4$; Q is optionally substituted aryl or heteroaryl, which act as matrix metalloprotease inhibitors, particularly diastereomerically pure β -hydroxy carboxylic acids, corresponding processes for the synthesis of and pharmaceutical compns. containing the compds. of the present invention. Compds. of the present invention are useful in the treatment of various inflammatory, autoimmune and allergic diseases, such as methods of treating asthma, rheumatoid arthritis, COPD, rhinitis, osteoarthritis, psoriatic arthritis, psoriasis, pulmonary fibrosis, wound healing disorders, pulmonary inflammation, acute respiratory distress syndrome, periodontitis, multiple sclerosis, gingivitis, atherosclerosis, neointimal proliferation, which leads to restenosis and ischemic heart failure, stroke, renal diseases, tumor metastasis, and other inflammatory disorders characterized by the over-expression and over-activation of a matrix metalloproteinase using the compds. Thus, (2S,3R)-3-hydroxy-2-[2-(4-oxo-1,2,3-benzotriazin-3(4H)-yl)ethyl]-5-(4-pyrimidin-5-yl-phenyl)pentanoic acid was prepared and tested in rats as metalloproteinase inhibitor. Pharmacokinetic screening assays for Matrix Metallo Proteinase (MMP 9/12) inhibitors, are reported. Compds. of the present invention can be selective over MMP-1 by > 100 fold.
- IT 87556-66-9, Cloticasone 90566-53-3, Fluticasone
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (preparation of uronic acid derivs. as metalloproteinase inhibitors)
- RN 87556-66-9 CAPLUS
- CN Androsta-1,4-diene-17-carbothioic acid,
 6,9-difluoro-11,17-dihydroxy-16-methyl-3-oxo-, S-(chloromethyl) ester,
 (6 α ,11 β ,16 α ,17 α)- (CA INDEX NAME)

Absolute stereochemistry.

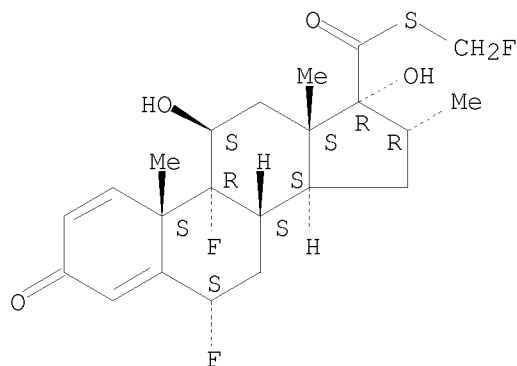
10/552,118



RN 90566-53-3 CAPLUS

CN Androsta-1,4-diene-17-carbothioic acid,
6,9-difluoro-11,17-dihydroxy-16-methyl-3-oxo-, S-(fluoromethyl) ester,
(6 α ,11 β ,16 α ,17 α)- (CA INDEX NAME)

Absolute stereochemistry.



IT 25952-53-8, EDCI

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of uronic acid derivs. as metalloproteinase inhibitors)

RN 25952-53-8 CAPLUS

CN 1,3-Propanediamine, N3-(ethylcarbonimidoyl)-N1,N1-dimethyl-, hydrochloride
(1:1) (CA INDEX NAME)

Et-N=C=N-(CH₂)₃-NMe₂

● HCl

L7 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2004:857616 CAPLUS

DOCUMENT NUMBER: 141:332364

TITLE: Process for the preparation of steroidal carbothioic acid derivatives and intermediates

INVENTOR(S): Loevli, Trond; Nygaard, Anne-mette; Reitstoen, Bjoern; Fivelstad, Magny

PATENT ASSIGNEE(S): Alpharma Aps, Den.

SOURCE: PCT Int. Appl., 40 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004087731	A1	20041014	WO 2004-DK242	20040402
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1466920	A1	20041013	EP 2003-7756	20030404
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AU 2004226318	A1	20041014	AU 2004-226318	20040402
AU 2004226318	B2	20080605		
CA 2530680	A1	20041014	CA 2004-2530680	20040402
EP 1611149	A1	20060104	EP 2004-725301	20040402
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
JP 2006522028	T	20060928	JP 2006-504347	20040402
NO 2005004636	A	20051227	NO 2005-4636	20051010
IN 2005CN02890	A	20070406	IN 2005-CN2890	20051103
US 20070270584	A1	20071122	US 2007-552118	20070413
PRIORITY APPLN. INFO.:			EP 2003-7756	A 20030404
			DK 2004-449	A 20040319
			WO 2004-DK242	W 20040402

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): CASREACT 141:332364; MARPAT 141:332364

AB Steroidal carboxthioc acids were prepared by reacting steroidal carboxylic acids or salts with a coupling agent alone or in conjunction with a coupling enhancer followed by reaction with a nucleophilic agent comprising a sulfur atom. Thus, 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-17 α -propionyloxyandrosta-1,,4-diene-17 β -carboxylic acid, prepared from flumetasone, in DMA was treated with EDC (1-ethyl-3-(3-dimethylaminopropyl)carbodiimide) and NHS (N-hydroxysuccinimide) followed by sodium hydrosulfide hydrate and then bromofluoromethane to give 92% S-fluoromethyl 6 α ,9 α -difluoro-11 β -hydroxy-16 α -methyl-3-oxo-

17 α -propionyloxyandrosta-1,4-diene-17 β -carbothioate
(fluticasone propionate).

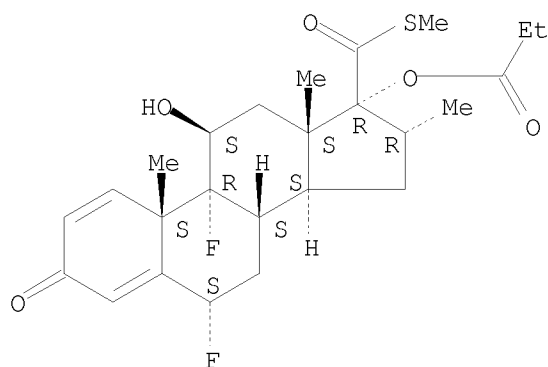
IT 73205-13-7P 80474-14-2P, Fluticasone propionate
80474-45-9P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
(Preparation)
(process for preparation of steroidal carbothioic acid derivs. and
intermediates)

RN 73205-13-7 CAPLUS

CN Androsta-1,4-diene-17-carbothioic acid,
6,9-difluoro-11-hydroxy-16-methyl-3-oxo-17-(1-oxopropoxy)-, S-methyl
ester, (6 α ,11 β ,16 α ,17 α)- (CA INDEX NAME)

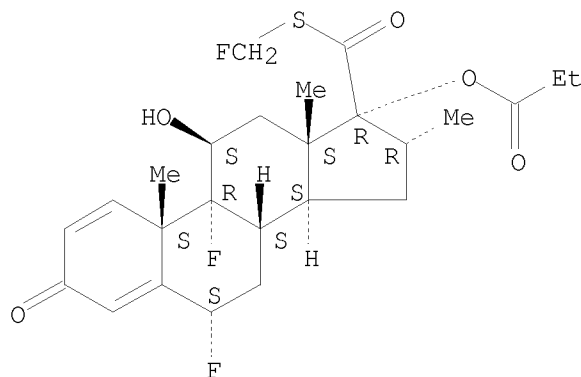
Absolute stereochemistry.



RN 80474-14-2 CAPLUS

CN Androsta-1,4-diene-17-carbothioic acid,
6,9-difluoro-11-hydroxy-16-methyl-3-oxo-17-(1-oxopropoxy)-,
S-(fluoromethyl) ester, (6 α ,11 β ,16 α ,17 α)- (CA
INDEX NAME)

Absolute stereochemistry.

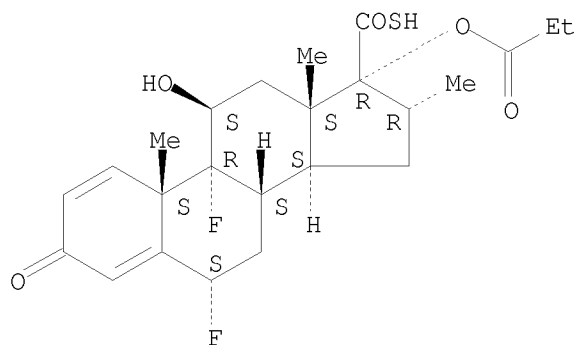


RN 80474-45-9 CAPLUS

CN Androsta-1,4-diene-17-carbothioic acid,
6,9-difluoro-11-hydroxy-16-methyl-3-oxo-17-(1-oxopropoxy)-,
(6 α ,11 β ,16 α ,17 α)- (CA INDEX NAME)

10/552,118

Absolute stereochemistry. Rotation (-).



IT 25952-53-8, Edc
RL: RGT (Reagent); RACT (Reactant or reagent)
(process for preparation of steroidal carbothioic acid derivs. and
intermediates)
RN 25952-53-8 CAPLUS
CN 1,3-Propanediamine, N3-(ethylcarbonimidoyl)-N1,N1-dimethyl-, hydrochloride
(1:1) (CA INDEX NAME)

Et-N=C=N-(CH₂)₃-NMe₂

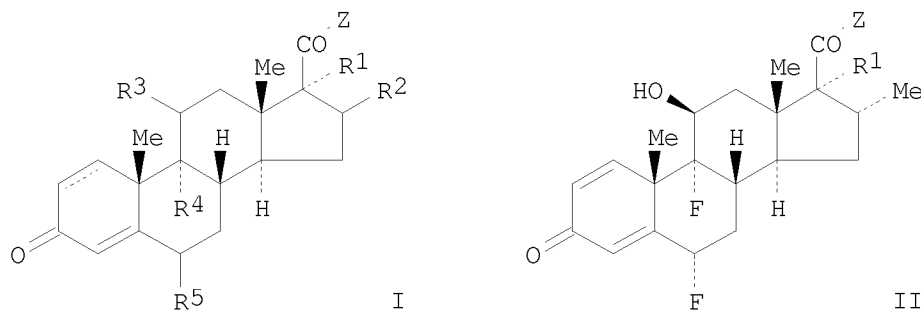
● HCl

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2004:837305 CAPLUS
 DOCUMENT NUMBER: 141:332363
 TITLE: Process for the preparation of steroidal
 17 β -carbothioates
 INVENTOR(S): Loevli, Trond; Nygard, Anne Mette; Reitstoen, Bjoern;
 Fivelstad, Magny
 PATENT ASSIGNEE(S): Alpharma Aps, Den.
 SOURCE: Eur. Pat. Appl., 18 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1466920	A1	20041013	EP 2003-7756	20030404
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AU 2004226318	A1	20041014	AU 2004-226318	20040402
AU 2004226318	B2	20080605		
CA 2530680	A1	20041014	CA 2004-2530680	20040402
WO 2004087731	A1	20041014	WO 2004-DK242	20040402
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1611149	A1	20060104	EP 2004-725301	20040402
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1798757	A	20060705	CN 2004-80015412	20040402
JP 2006522028	T	20060928	JP 2006-504347	20040402
NO 2005004636	A	20051227	NO 2005-4636	20051010
IN 2005CN02890	A	20070406	IN 2005-CN2890	20051103
US 20070270584	A1	20071122	US 2007-552118	20070413
PRIORITY APPLN. INFO.:			EP 2003-7756	A 20030404
			DK 2004-449	A 20040319
			WO 2004-DK242	W 20040402
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT				
OTHER SOURCE(S): MARPAT 141:332363				
GI				



AB A novel method was disclosed for the conversion of steroidal 17β-carboxylic acids I (Z = OH) to the corresponding carbothioates I [R1 = H, OH, acyloxy; R2 = H, α-OH, α-, β-alkyl; R1R2 = fused 1,3-dioxolane ring of the form -OCR7R8O-; R3 = OH, protected hydroxyl; R4 = H, halogen; R3R4 = bond, -O- (epoxide); R5 = H, halogen; R7, R8 = H, alkyl; Z = SCH2F, SCH2Br, S(CH2)2F] including fluticasone propionate II (R1 = COCH2Me, Z = SCH2F), via novel in situ generated 17β-carboxy imidazolyl- or succinimidyl esters. Thus, flumetasone II (R1 = OH, Z = CH2OH) was oxidized using periodic acid to form the corresponding acid II (R1 = Z = OH) in 98% yield. The the acid was esterified with MeCH2COCl using NEt3 to give 17α-propionate II (R1 = OCOCH2Me, Z = OH) in 99% yield, and subsequent treatment of the 17α-propionate with NHS and FCH2Br gave fluticasone propionate in 75% yield.

IT 25952-53-8, EDC

RL: RGT (Reagent); RACT (Reactant or reagent)

(process for the preparation of steroidal 17-carbothioates)

RN 25952-53-8 CAPLUS

CN 1,3-Propanediamine, N3-(ethylcarbonimidoyl)-N1,N1-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)

Et-N=C=N-(CH2)3-NMe2

● HCl

IT 73205-13-7P 80474-14-2P, Fluticasone propionate

80474-45-9P

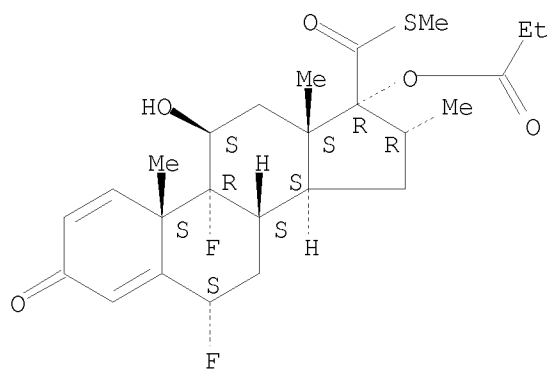
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(process for the preparation of steroidal 17β-carbothioates)

RN 73205-13-7 CAPLUS

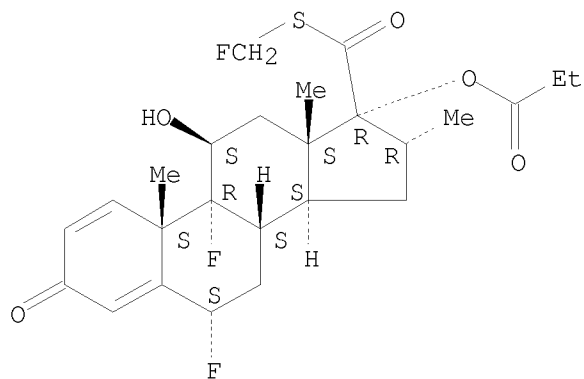
CN Androsta-1,4-diene-17-carbothioic acid, 6,9-difluoro-11-hydroxy-16-methyl-3-oxo-17-(1-oxopropoxy)-, S-methyl ester, (6α,11β,16α,17α)- (CA INDEX NAME)

Absolute stereochemistry.



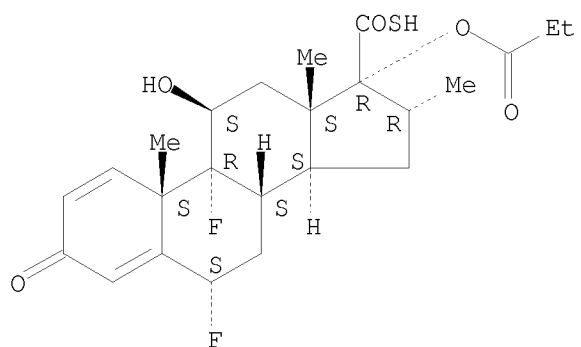
RN 80474-14-2 CAPLUS
 CN Androsta-1,4-diene-17-carbothioic acid,
 6,9-difluoro-11-hydroxy-16-methyl-3-oxo-17-(1-oxopropoxy)-,
 S-(fluoromethyl) ester, (6 α ,11 β ,16 α ,17 α)- (CA
 INDEX NAME)

Absolute stereochemistry.



RN 80474-45-9 CAPLUS
 CN Androsta-1,4-diene-17-carbothioic acid,
 6,9-difluoro-11-hydroxy-16-methyl-3-oxo-17-(1-oxopropoxy)-,
 (6 α ,11 β ,16 α ,17 α)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT:

3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN

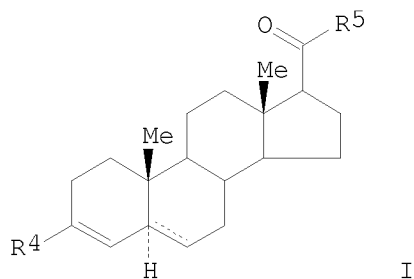
ACCESSION NUMBER: 1993:124875 CAPLUS
 DOCUMENT NUMBER: 118:124875
 ORIGINAL REFERENCE NO.: 118:21669a,21672a
 TITLE: Preparation of
 17-(ureidocarbonyl)androsta-3,5-diene-3-carboxylates
 and analogs as testosterone 5 α -reductase
 inhibitors
 INVENTOR(S): Panzeri, Achille; Nesi, Marcella; Di Salle, Enrico
 PATENT ASSIGNEE(S): Farmitalia Carlo Erba S.r.l., Italy
 SOURCE: PCT Int. Appl., 43 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9220700	A1	19921126	WO 1992-EP1153	19920522
W: AU, CA, CS, FI, HU, JP, KR, NO, RU				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
US 5212166	A	19930518	US 1992-886574	19920521
IL 101947	A	19960119	IL 1992-101947	19920521
CA 2087953	A1	19921125	CA 1992-2087953	19920522
EP 517047	A1	19921209	EP 1992-108670	19920522
R: PT				
AU 9217781	A	19921230	AU 1992-17781	19920522
AU 655280	B2	19941215		
ZA 9203758	A	19930127	ZA 1992-3758	19920522
EP 540717	A1	19930512	EP 1992-910992	19920522
EP 540717	B1	19970723		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE				
HU 64083	A2	19931129	HU 1993-176	19920522
JP 06500342	T	19940113	JP 1992-509789	19920522
JP 3226919	B2	20011112		
CZ 281309	B6	19960814	CZ 1993-265	19920522
AT 155792	T	19970815	AT 1992-910992	19920522
ES 2106185	T3	19971101	ES 1992-910992	19920522
RU 2104283	C1	19980210	RU 1993-4939	19920522
CN 1067057	A	19921216	CN 1992-103919	19920523
CN 1035055	C	19970604		
NO 9300244	A	19930127	NO 1993-244	19930125
PRIORITY APPLN. INFO.:			IT 1991-MI1432	A 19910524
			WO 1992-EP1153	A 19920522

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 118:124875

GI



AB Title compds. [I; R4 = COR; R = OH, alkoxy, (di)(alkyl)amino, alkanoyloxymethoxy, OCH₂CONH₂, etc.; R5 = NR₁C(:Y)NR₂R₃; R₁-R₃ = H, (cyclo)alkyl, aryl, etc.; NR₂R₃ = heterocyclyl; Y = O, S; dashed line = optional bond] were prepared. Thus, androst-4-en-3-one-17 β -carboxylic acid was condensed with (Me₂CHNH)₂CO and the product treated with 2,6-di-tert-butyl-4-methylpyridine and (CF₃SO₂)₂O to give I [R5 = CON(CHMe₂)CONHCHMe₂, dashed line = bond] (II; R4 = OSO₂CF₃) which was stirred overnight under CO in DMF containing MeOH, Et₃N, and (Ph₃P)₂Pd(OAc)₂ to give, after saponification, II (R4 = CO₂H). The latter had IC₅₀ of 3 nM against testosterone 5 α -reductase in vitro.

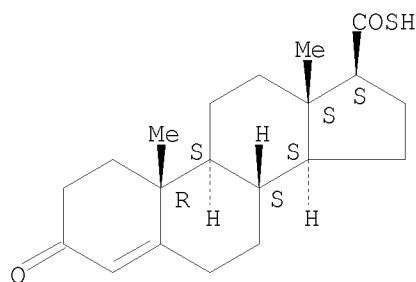
IT 146175-30-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of testosterone 5 α -reductase inhibitors)

RN 146175-30-6 CAPLUS

CN Androst-4-ene-17-carbothioic acid, 3-oxo-, (17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

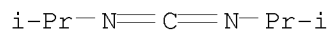


IT 693-13-0, N,N'-Diisopropylcarbodiimide 146175-29-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of testosterone 5 α -reductase inhibitors)

RN 693-13-0 CAPLUS

CN 2-Propanamine, N,N'-methanetetraylbis- (CA INDEX NAME)

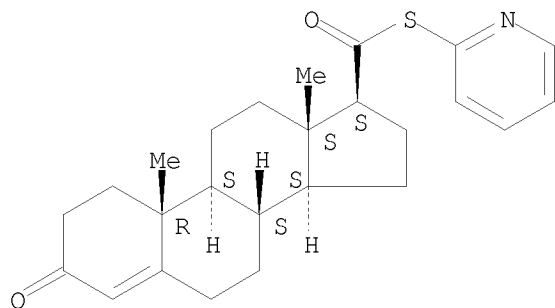


10/552,118

RN 146175-29-3 CAPLUS

CN Androst-4-ene-17-carbothioic acid, 3-oxo-, S-2-pyridinyl ester,
(17 β)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT:	8	THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)
REFERENCE COUNT:	3	THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT